



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 10:08 am GMT

PDB ID : 2P90
Title : The crystal structure of a protein of unknown function from *Corynebacterium glutamicum* ATCC 13032
Authors : Zhang, R.; Duggan, E.; Gu, M.; Joachimiak, A.; Midwest Center for Structural Genomics (MCSG)
Deposited on : 2007-03-23
Resolution : 2.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

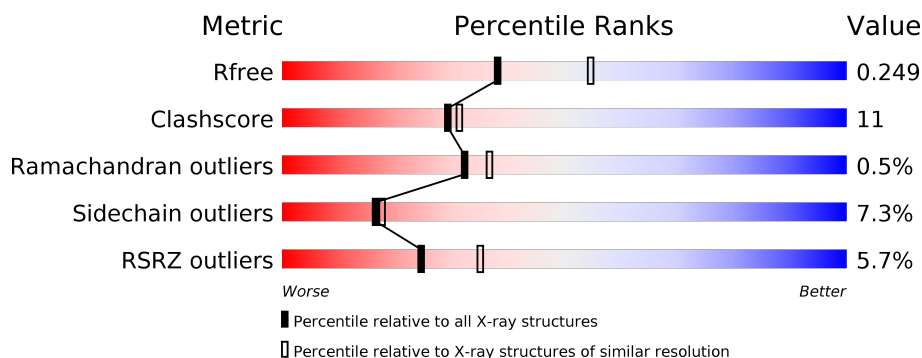
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1522 (2.38-2.34)
Clashscore	112137	1626 (2.38-2.34)
Ramachandran outliers	110173	1605 (2.38-2.34)
Sidechain outliers	110143	1606 (2.38-2.34)
RSRZ outliers	101464	1528 (2.38-2.34)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	319	<div> <div>8%</div> <div> <div></div> <div>68%</div> <div>13%</div> <div>•</div> <div>16%</div> </div> </div>
1	B	319	<div> <div>3%</div> <div> <div></div> <div>65%</div> <div>15%</div> <div>5%</div> <div>15%</div> </div> </div>
1	C	319	<div> <div>4%</div> <div> <div></div> <div>64%</div> <div>15%</div> <div>•</div> <div>17%</div> </div> </div>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6595 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Hypothetical protein Cgl1923.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	269	Total	C	N	O	S	0	0	0
			2092	1303	364	416	9			
1	B	271	Total	C	N	O	S	0	0	0
			2109	1314	369	417	9			
1	C	266	Total	C	N	O	S	0	0	0
			2068	1289	361	409	9			

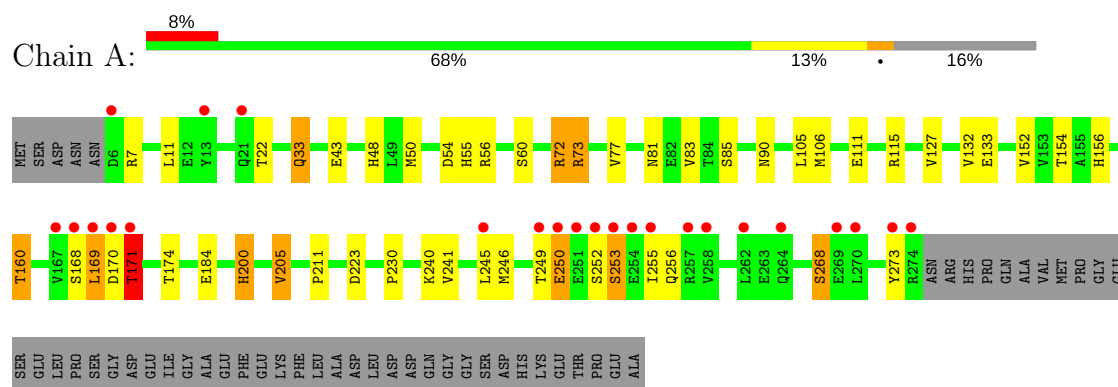
- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	125	Total	O	0	0
			125	125		
2	B	107	Total	O	0	0
			107	107		
2	C	94	Total	O	0	0
			94	94		

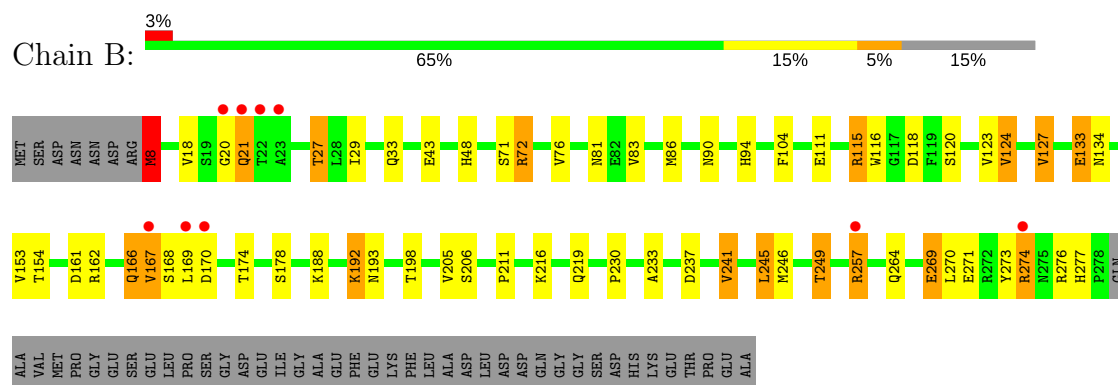
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

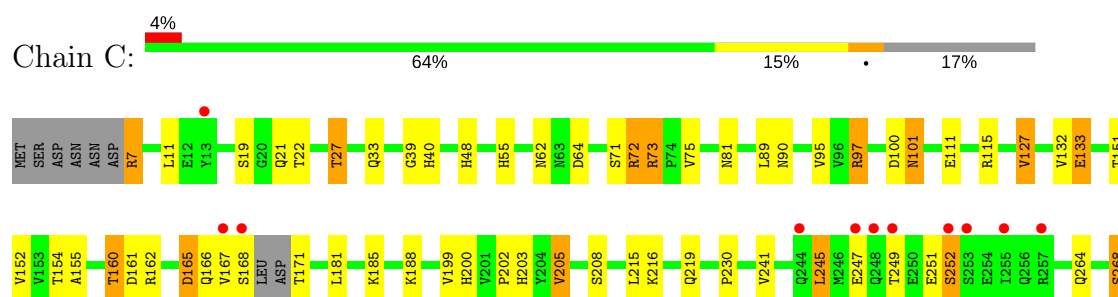
• Molecule 1: Hypothetical protein Cgl1923



• Molecule 1: Hypothetical protein Cgl1923



• Molecule 1: Hypothetical protein Cgl1923



R272	ASN
Y273	ARG
R274	HIS
	PRO
	GLN
	ALA
	VAL
	MET
	PRO
	GLY
	GLU
	SER
	GLU
	LEU
	PRO
	SER
	GLY
	ASP
	GLU
	ILE
	GLY
	ALA
	GLU
	PHE
	GLU
	LYS
	PHE
	LEU
	ALA
	ASP
	LEU
	ASP
	ASP
	GLN
	GLY
	GLY
	SER
	ASP
	HIS
	LYS
	GLU
	THR
	PRO
	GLU
	ALA

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.83Å 113.35Å 117.37Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.65 – 2.35 44.40 – 2.34	Depositor EDS
% Data completeness (in resolution range)	99.8 (81.65-2.35) 99.4 (44.40-2.34)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.18 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.193 , 0.251 0.192 , 0.249	Depositor DCC
R_{free} test set	2420 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	44.8	Xtriage
Anisotropy	0.424	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.013 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6595	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.78	2/2132 (0.1%)	0.86	6/2900 (0.2%)
1	B	0.80	4/2151 (0.2%)	0.84	5/2927 (0.2%)
1	C	0.79	0/2107	0.95	10/2864 (0.3%)
All	All	0.79	6/6390 (0.1%)	0.89	21/8691 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	43	GLU	CD-OE1	7.27	1.33	1.25
1	A	43	GLU	CD-OE1	6.94	1.33	1.25
1	B	43	GLU	CG-CD	6.46	1.61	1.51
1	B	269	GLU	CG-CD	6.21	1.61	1.51
1	A	43	GLU	CG-CD	6.08	1.61	1.51
1	B	43	GLU	CD-OE2	5.80	1.32	1.25

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	72	ARG	NE-CZ-NH2	-13.89	113.35	120.30
1	C	73	ARG	NE-CZ-NH2	-12.49	114.06	120.30
1	C	115	ARG	NE-CZ-NH2	-12.29	114.15	120.30
1	A	115	ARG	NE-CZ-NH2	-11.02	114.79	120.30
1	C	73	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	A	73	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	72	ARG	NE-CZ-NH2	-8.31	116.15	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	B	115	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	C	72	ARG	NE-CZ-NH1	7.51	124.06	120.30
1	B	115	ARG	NE-CZ-NH1	7.30	123.95	120.30
1	A	73	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	B	8	MET	CG-SD-CE	6.94	111.30	100.20
1	C	115	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	A	72	ARG	NE-CZ-NH1	6.89	123.75	120.30
1	C	72	ARG	CG-CD-NE	-6.66	97.82	111.80
1	B	72	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	A	72	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	C	165	ASP	CB-CG-OD1	5.72	123.45	118.30
1	C	89	LEU	CA-CB-CG	5.65	128.28	115.30
1	C	64	ASP	CB-CG-OD1	5.60	123.34	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	171	THR	Peptide

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2092	0	2048	45	0
1	B	2109	0	2064	53	0
1	C	2068	0	2028	51	0
2	A	125	0	0	13	0
2	B	107	0	0	14	0
2	C	94	0	0	17	0
All	All	6595	0	6140	134	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (134) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:GLN:HG2	2:B:403:HOH:O	1.32	1.23
1:C:152:VAL:HG13	1:C:167:VAL:HG21	1.39	1.03
1:A:106:MET:SD	2:A:433:HOH:O	2.19	0.99
1:C:90:ASN:HB2	2:C:333:HOH:O	1.59	0.98
1:C:152:VAL:HG13	1:C:167:VAL:CG2	1.97	0.95
1:A:90:ASN:HB2	2:A:403:HOH:O	1.66	0.93
1:B:72:ARG:NH2	1:B:111:GLU:O	2.02	0.90
1:B:211:PRO:HD2	1:B:241:VAL:HG11	1.53	0.90
1:C:7:ARG:HG2	2:C:364:HOH:O	1.71	0.87
1:B:8:MET:N	2:B:414:HOH:O	2.07	0.87
1:C:203:HIS:HB3	2:C:371:HOH:O	1.76	0.86
1:B:18:VAL:O	1:B:18:VAL:HG12	1.78	0.83
1:C:72:ARG:NH2	1:C:111:GLU:O	2.13	0.81
1:B:245:LEU:O	1:B:249:THR:HG22	1.80	0.80
1:C:152:VAL:CG1	1:C:167:VAL:HG21	2.11	0.80
1:B:90:ASN:HB2	2:B:375:HOH:O	1.84	0.76
1:A:211:PRO:HD2	1:A:241:VAL:HG11	1.67	0.76
1:B:233:ALA:HA	2:B:426:HOH:O	1.84	0.76
1:A:240:LYS:HE2	2:A:427:HOH:O	1.85	0.75
1:A:72:ARG:NH2	1:A:111:GLU:O	2.20	0.74
1:A:77:VAL:HG22	1:B:174:THR:HG22	1.69	0.73
1:A:168:SER:HB2	1:A:169:LEU:HA	1.71	0.73
1:B:133:GLU:OE1	1:B:162:ARG:NH1	2.16	0.73
1:B:76:VAL:HG21	1:C:181:LEU:HD13	1.74	0.70
1:A:77:VAL:HB	1:A:85:SER:HB3	1.76	0.68
1:B:167:VAL:O	1:B:167:VAL:HG12	1.94	0.67
1:C:7:ARG:CG	2:C:364:HOH:O	2.33	0.66
1:A:169:LEU:HB2	1:C:81:ASN:OD1	1.95	0.66
1:A:160:THR:CG2	2:A:410:HOH:O	2.43	0.66
1:A:246:MET:O	1:A:249:THR:HG22	1.96	0.66
1:C:27:THR:HG22	2:C:341:HOH:O	1.95	0.66
1:B:33:GLN:CG	2:B:403:HOH:O	2.12	0.65
1:B:154:THR:HG22	1:B:168:SER:HA	1.79	0.64
1:C:81:ASN:HB3	2:C:361:HOH:O	1.97	0.64
1:C:171:THR:HB	2:C:387:HOH:O	1.98	0.64
1:B:18:VAL:O	1:B:18:VAL:CG1	2.47	0.63
1:C:165:ASP:OD2	1:C:216:LYS:NZ	2.22	0.63
1:B:237:ASP:O	1:B:241:VAL:HG12	1.98	0.63
1:A:73:ARG:HH22	1:B:111:GLU:CD	2.02	0.63
1:B:270:LEU:O	1:B:274:ARG:HG2	2.00	0.62
1:A:33:GLN:HG2	2:A:415:HOH:O	1.98	0.62
1:C:166:GLN:HE21	1:C:168:SER:HB2	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:GLN:OE1	2:C:381:HOH:O	2.16	0.60
1:B:166:GLN:HG2	1:B:166:GLN:O	2.01	0.60
1:A:160:THR:HG22	2:A:410:HOH:O	2.00	0.60
1:B:192:LYS:HE3	2:B:398:HOH:O	2.01	0.60
1:C:251:GLU:O	1:C:252:SER:HB2	2.02	0.59
1:A:170:ASP:N	1:C:81:ASN:OD1	2.28	0.59
1:A:205:VAL:HG22	2:A:404:HOH:O	2.02	0.58
1:C:22:THR:HA	2:C:378:HOH:O	2.02	0.58
1:A:171:THR:HA	2:C:406:HOH:O	2.02	0.57
1:A:253:SER:HA	2:A:352:HOH:O	2.05	0.57
1:C:151:THR:CG2	1:C:199:VAL:CG2	2.82	0.56
1:B:94:HIS:HD2	2:B:405:HOH:O	1.89	0.56
1:A:50:MET:HG3	1:A:55:HIS:CD2	2.41	0.56
1:A:156:HIS:HE1	1:A:184:GLU:OE1	1.90	0.55
1:B:8:MET:N	2:B:390:HOH:O	2.40	0.55
1:A:48:HIS:HE1	1:A:230:PRO:O	1.90	0.54
1:C:27:THR:HG21	2:C:353:HOH:O	2.05	0.54
1:B:94:HIS:CD2	2:B:405:HOH:O	2.59	0.54
1:C:203:HIS:CB	2:C:371:HOH:O	2.43	0.54
1:C:100:ASP:O	1:C:101:ASN:HB2	2.08	0.53
1:C:215:LEU:O	1:C:219:GLN:HG3	2.08	0.53
1:A:169:LEU:CB	1:C:81:ASN:OD1	2.57	0.53
1:A:168:SER:CB	1:A:169:LEU:HA	2.38	0.52
1:A:7:ARG:HA	2:A:434:HOH:O	2.10	0.52
1:A:111:GLU:OE2	1:C:73:ARG:NH2	2.40	0.52
1:C:151:THR:HG21	1:C:199:VAL:CG2	2.40	0.51
1:B:120:SER:O	1:B:124:VAL:HG13	2.11	0.51
1:B:257:ARG:HB2	1:B:257:ARG:NH1	2.25	0.51
1:C:216:LYS:NZ	2:C:412:HOH:O	2.40	0.50
1:A:73:ARG:NH2	1:B:111:GLU:OE2	2.43	0.50
1:B:167:VAL:CG1	1:B:167:VAL:O	2.60	0.49
1:C:205:VAL:HG21	1:C:245:LEU:HD21	1.94	0.49
1:A:154:THR:OG1	1:A:200:HIS:HE1	1.95	0.49
1:A:174:THR:HG23	1:C:75:VAL:CG1	2.43	0.49
1:B:169:LEU:HB2	1:B:273:TYR:CD1	2.48	0.49
1:B:48:HIS:HE1	1:B:230:PRO:O	1.96	0.49
1:C:39:GLY:HA2	1:C:208:SER:O	2.13	0.49
1:A:273:TYR:HB2	2:A:422:HOH:O	2.13	0.48
1:C:19:SER:H	1:C:97:ARG:HH12	1.58	0.48
1:B:27:THR:HG22	2:B:362:HOH:O	2.13	0.48
1:C:62:ASN:HB2	2:C:373:HOH:O	2.13	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:134:ASN:HD22	1:B:193:ASN:HB3	1.79	0.48
1:A:156:HIS:CE1	1:A:184:GLU:OE1	2.67	0.48
1:C:160:THR:HG23	1:C:166:GLN:HE22	1.79	0.48
1:C:27:THR:HG23	2:C:358:HOH:O	2.13	0.48
1:A:170:ASP:C	1:A:171:THR:HG22	2.34	0.47
1:B:169:LEU:HB2	1:B:273:TYR:HD1	1.79	0.47
1:A:83:VAL:O	1:B:188:LYS:HE2	2.14	0.47
1:C:202:PRO:HD3	2:C:404:HOH:O	2.13	0.47
1:C:154:THR:HG23	1:C:200:HIS:CE1	2.49	0.47
1:C:133:GLU:HG3	2:C:341:HOH:O	2.14	0.47
1:A:252:SER:HB3	1:A:255:ILE:HD12	1.96	0.47
1:A:256:GLN:HB2	2:A:352:HOH:O	2.14	0.47
1:A:111:GLU:CD	1:C:73:ARG:HH22	2.18	0.46
1:A:169:LEU:H	1:A:169:LEU:HG	1.61	0.46
1:B:83:VAL:O	1:C:188:LYS:HE2	2.16	0.45
1:C:152:VAL:HG13	1:C:167:VAL:HG23	1.93	0.45
1:A:174:THR:HG23	1:C:75:VAL:HG13	1.98	0.45
1:B:216:LYS:HA	1:B:216:LYS:HD2	1.79	0.45
1:B:81:ASN:ND2	1:C:155:ALA:O	2.50	0.45
1:B:169:LEU:HD21	1:B:276:ARG:HH11	1.82	0.44
1:B:115:ARG:NH1	1:B:118:ASP:OD2	2.45	0.44
1:A:170:ASP:C	1:A:171:THR:CG2	2.86	0.44
1:B:216:LYS:HD2	1:B:219:GLN:HE21	1.81	0.44
1:B:29:ILE:HD12	1:B:104:PHE:CD1	2.53	0.44
1:B:274:ARG:HD3	2:B:373:HOH:O	2.17	0.44
1:A:127:VAL:HG13	1:A:132:VAL:HB	2.00	0.44
1:C:55:HIS:HA	1:C:95:VAL:O	2.17	0.44
1:C:133:GLU:OE1	1:C:162:ARG:NH1	2.28	0.43
1:A:54:ASP:HB3	1:A:56:ARG:HH12	1.83	0.43
1:C:48:HIS:HE1	1:C:230:PRO:O	2.01	0.43
1:B:116:TRP:CH2	1:B:178:SER:HA	2.53	0.43
1:C:40:HIS:N	1:C:40:HIS:CD2	2.87	0.43
1:B:20:GLY:O	1:B:21:GLN:HB3	2.18	0.43
1:B:21:GLN:HG2	1:B:21:GLN:O	2.19	0.43
1:A:160:THR:HG21	2:A:380:HOH:O	2.18	0.43
1:C:127:VAL:HB	1:C:132:VAL:HB	2.00	0.42
1:A:50:MET:HG3	1:A:55:HIS:NE2	2.33	0.42
1:B:246:MET:HG2	2:B:399:HOH:O	2.19	0.42
1:A:171:THR:HA	2:A:335:HOH:O	2.19	0.42
1:C:264:GLN:O	1:C:268:SER:HB3	2.19	0.42
1:A:250:GLU:H	1:A:250:GLU:HG2	1.79	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:GLN:HG2	2:B:401:HOH:O	2.19	0.41
1:B:169:LEU:HD13	1:B:277:HIS:NE2	2.36	0.41
2:B:357:HOH:O	1:C:185:LYS:HE3	2.19	0.41
1:C:100:ASP:O	1:C:101:ASN:CB	2.68	0.41
1:B:76:VAL:HG12	1:B:86:MET:HG3	2.03	0.41
1:A:81:ASN:HD21	1:B:170:ASP:HB2	1.86	0.41
1:B:271:GLU:HG2	1:B:274:ARG:HH21	1.86	0.40
1:B:123:VAL:O	1:B:127:VAL:HG13	2.20	0.40
1:B:257:ARG:HB2	1:B:257:ARG:CZ	2.52	0.40
1:B:153:VAL:HA	1:B:198:THR:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	267/319 (84%)	257 (96%)	9 (3%)	1 (0%)	38	44
1	B	269/319 (84%)	259 (96%)	8 (3%)	2 (1%)	25	27
1	C	262/319 (82%)	251 (96%)	10 (4%)	1 (0%)	38	44
All	All	798/957 (83%)	767 (96%)	27 (3%)	4 (0%)	32	37

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	21	GLN
1	C	252	SER
1	A	268	SER
1	B	167	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	234/276 (85%)	217 (93%)	17 (7%)	16	18
1	B	236/276 (86%)	219 (93%)	17 (7%)	17	18
1	C	231/276 (84%)	214 (93%)	17 (7%)	16	17
All	All	701/828 (85%)	650 (93%)	51 (7%)	16	18

All (51) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	11	LEU
1	A	22	THR
1	A	33	GLN
1	A	60	SER
1	A	105	LEU
1	A	133	GLU
1	A	152	VAL
1	A	160	THR
1	A	169	LEU
1	A	171	THR
1	A	200	HIS
1	A	205	VAL
1	A	223	ASP
1	A	245	LEU
1	A	250	GLU
1	A	253	SER
1	A	268	SER
1	B	8	MET
1	B	27	THR
1	B	71	SER
1	B	124	VAL
1	B	127	VAL
1	B	133	GLU
1	B	161	ASP
1	B	166	GLN
1	B	192	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	205	VAL
1	B	206	SER
1	B	241	VAL
1	B	245	LEU
1	B	249	THR
1	B	257	ARG
1	B	269	GLU
1	B	274	ARG
1	C	7	ARG
1	C	11	LEU
1	C	21	GLN
1	C	27	THR
1	C	71	SER
1	C	97	ARG
1	C	101	ASN
1	C	127	VAL
1	C	133	GLU
1	C	160	THR
1	C	161	ASP
1	C	205	VAL
1	C	241	VAL
1	C	245	LEU
1	C	247	GLU
1	C	249	THR
1	C	268	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	HIS
1	A	134	ASN
1	A	156	HIS
1	A	200	HIS
1	B	48	HIS
1	B	81	ASN
1	B	134	ASN
1	B	156	HIS
1	B	219	GLN
1	B	256	GLN
1	C	21	GLN
1	C	48	HIS
1	C	134	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	166	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	269/319 (84%)	0.48	24 (8%) 10 15	33, 44, 96, 122	0
1	B	271/319 (84%)	0.11	9 (3%) 47 59	34, 49, 71, 86	0
1	C	266/319 (83%)	0.11	13 (4%) 30 42	31, 45, 90, 102	0
All	All	806/957 (84%)	0.23	46 (5%) 24 35	31, 46, 89, 122	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	TYR	7.4
1	B	169	LEU	7.3
1	A	270	LEU	6.3
1	A	254	GLU	5.3
1	A	249	THR	5.2
1	A	169	LEU	5.0
1	A	171	THR	4.3
1	A	255	ILE	4.2
1	A	262	LEU	4.1
1	C	168	SER	4.1
1	A	170	ASP	3.8
1	A	13	TYR	3.8
1	A	257	ARG	3.7
1	C	167	VAL	3.7
1	A	252	SER	3.5
1	C	272	ARG	3.4
1	A	264	GLN	3.3
1	B	167	VAL	3.3
1	A	168	SER	3.2
1	B	21	GLN	3.2
1	A	258	VAL	3.1
1	A	167	VAL	3.0
1	C	253	SER	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	257	ARG	3.0
1	B	23	ALA	2.9
1	C	273	TYR	2.9
1	A	274	ARG	2.8
1	A	6	ASP	2.7
1	B	22	THR	2.5
1	B	274	ARG	2.5
1	C	13	TYR	2.4
1	C	248	GLN	2.4
1	A	253	SER	2.4
1	B	170	ASP	2.3
1	C	255	ILE	2.3
1	A	245	LEU	2.3
1	B	257	ARG	2.3
1	C	249	THR	2.3
1	A	21	GLN	2.3
1	C	252	SER	2.3
1	C	244	GLN	2.3
1	A	251	GLU	2.2
1	B	20	GLY	2.2
1	C	247	GLU	2.1
1	A	269	GLU	2.1
1	A	250	GLU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.